SIMTarget 1.0

User's guide

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1 Introduction

Ion beam analysis techniques are often used for the determination of elemental concentration depth profiles of various samples. The final results rely on simulations, fitting and calculations, made by dedicated codes written for specific techniques [1]. Amongst the different softwares available, SIMNRA [2] is one of the more powerful codes used to simulate experimental spectra obtained by Rutherford Backscattering Spectroscopy (RBS), Elastic Recoil Detection Analysis (ERDA), Nuclear Reaction Analysis (NRA) or Medium Energy Ion Scattering (MEIS). The best agreement between the theoretical and experimental results is obtained by adjusting the composition of the SIMNRA target file. When the structure of the sample under analysis becomes more complicated, the target file has to be manually sliced into several layers, which can rapidly become tedious.

SIMTarget code has then been designed in order to easily generate all SIMNRA target files regardless to the sample complexity. It is able to model the diffusion between two layers, as well as the presence of dopants within the sample. A graphical display shows the depth distribution of each element, which is very useful to adjust the target composition during simulations.

2 Installation

SIMTarget code has been written in Visual Basic for Application (VBA) within Microsoft Excel 2003. The execution of the SIMTarget macros has to be enabled in Excel in order to run this program. To do this, select “Tools” menu, point “Macro”, click “Security…” and then choose the “Medium” level of security. At this level, a dialog box will ask if you want to enable the macros when opening the SIMTarget 1.0.xls file. Select “Enable macros” and then SIMTarget is ready for use.

3 Using SIMTarget

3.1 Overview of SIMTarget

SIMTarget 1.0.xls is composed of eleven Excel spreadsheets. A short description of each is given below:

- Target description: This interactive sheet allows the user to describe the target material step by step as detail in the section 3.2.

- Target simulation: Contains the information about any dopant present (i.e. parameters of Gaussian or Lorentzian curves) and diffusion process (i.e. width of Boltzmann distribution). The general graph showing the depth profile of each element of the target is also included on this sheet. Modify or copy this graph requires to unprotect the "Target simulation" sheet. Deleting this graph may cause errors in the operation of SIMTarget.

- Concentrations: Allows determination of the mean concentration of any dopant between depths x_1 and x_2 chosen by the user.

- Curves: Contains the depth profile of each Gaussian or Lorentzian curve for any dopants present.

- Results: This sheet is completed automatically by SIMTarget, giving the depth profile of each target element.

- Elements: Contains information about all the elements available in SIMNRA code. As this is used to generate the SIMNRA target file, the contents of this sheet can not be modified under any circumstances.

- Isotopes: Contains information about all isotopes available in SIMNRA code. As this is used to generate the SIMNRA target file, the contents of this sheet can not be modified under any circumstances.

- Alloys: This interactive sheet allows the user to define any alloys that you wish to use in the target description (see section 3.5.2).

- Output parameters: Contains all the information required to reset the program or to recall parameters of a previous simulation. The contents of this sheet can not be modified under any circumstances.

- Target Format: Contains information about the format of the SIMNRA target file. The contents of this sheet can not be modified under any circumstances.

- Graph1: If any dopants are used in the target description, this graph is duplicated in order to present the depth profile of each Gaussian or Lorentzian curve. It must never be deleted.

Many of these sheets are protected in order to avoid any involuntary modification of contents. Unprotecting and modifying these sheets may cause errors in the operation of SIMTarget. Changing the names of the sheets can also cause errors.

3.2 ***Describing a target***

The target description is entirely performed within the interactive “Target description” sheet. The contents of this sheet will be automatically updated after each describing step. Basically, users must insert data to complete the cells appearing in grey before continuing to the next step.

First of all, “Thick” or “Multilayer” sample has to be selected. Thick sample is specifically used to model ion implantation into a substrate, while Multilayer sample is used to simulate all other samples. Move the mouse over the box at the right of cell A1, and tick the desired type of sample (Figure 1).

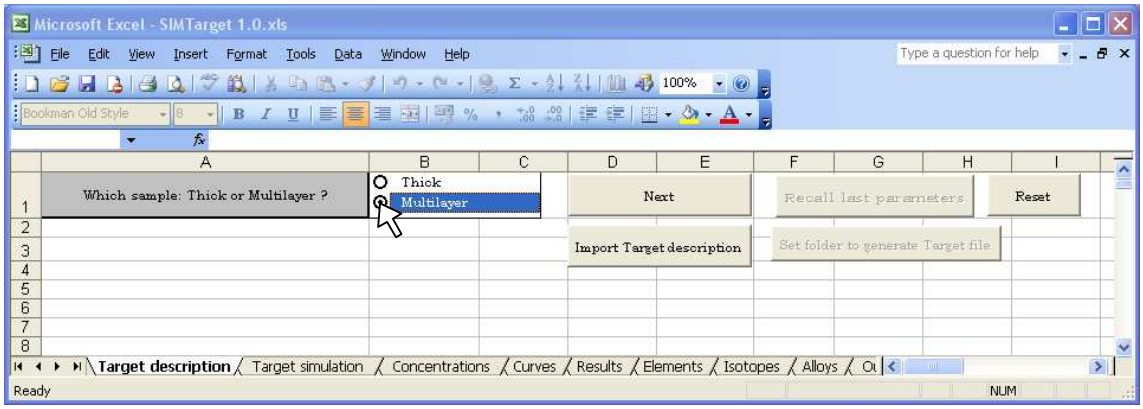


Figure 1: Type of sample selection.

Information about the SIMNRA target file will appear when hitting the “Next” button (Figure 2). Version 6.04 of the SIMNRA program is automatically selected and a dialog box simulating Windows Explorer is opened, in order to select the folder in which the target file will be created. If another version of SIMNRA is used, select this within the item list of cell B5. Specify the name of the target file and click the “Next” button again. The following options appearing on the screen are specific for Thick samples or Multilayer samples and are described in the sections 3.2.1 and 3.2.2, respectively. Note that the SIMNRA version, directory and name of the target file will be saved when the target description is completed, and automatically recalled during the future uses of SIMTarget code.

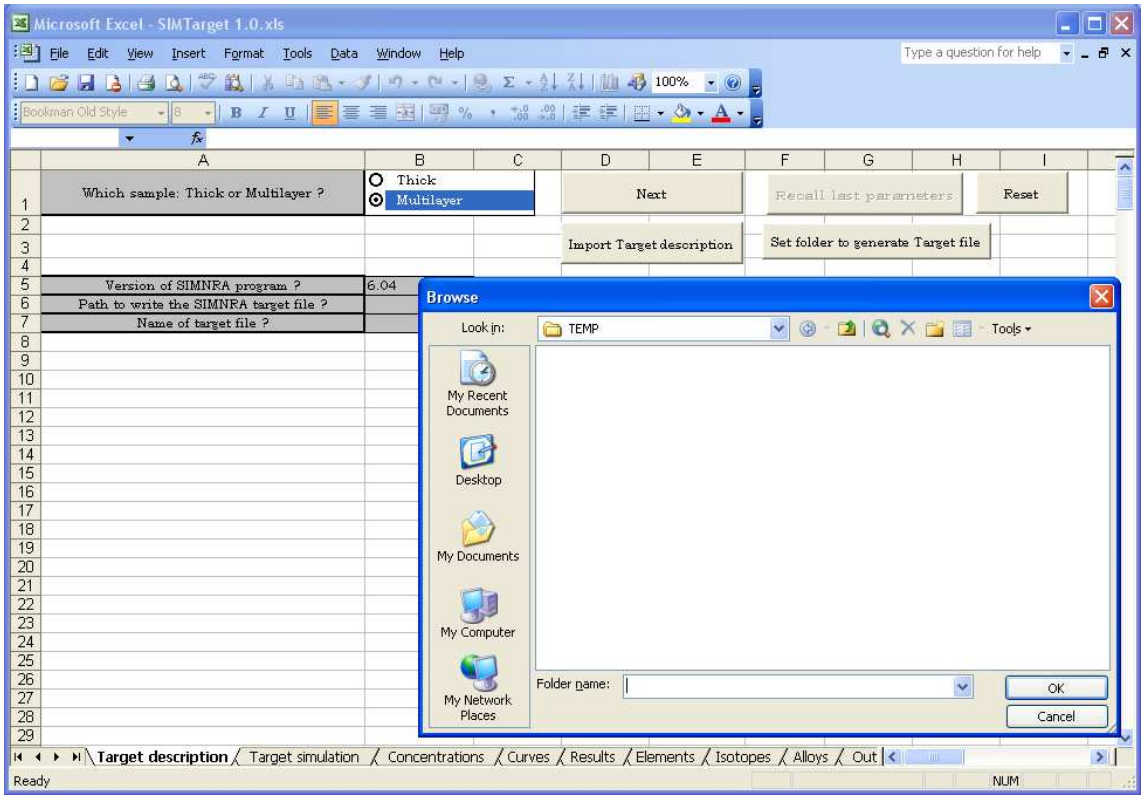


Figure 2: SIMNRA target file information.

3.2.1 Thick samples

Insert details of the thickness and the number of elements of the contamination layer. Specify the nature of each element by writing its chemical symbol with the keyboard. A dialog box will warn you if the element or the isotope chosen is not available in the SIMNRA code. Alloys can also be used if they have previously been defined in the “Alloys” sheet (see section 3.5.2). If the surface contamination contains several elements, the concentration of the last constituent will be automatically determined by the program. If no contamination layer is required, set the thickness and the number of elements to 0. When all grey cells are completed, press the “Confirm” button.

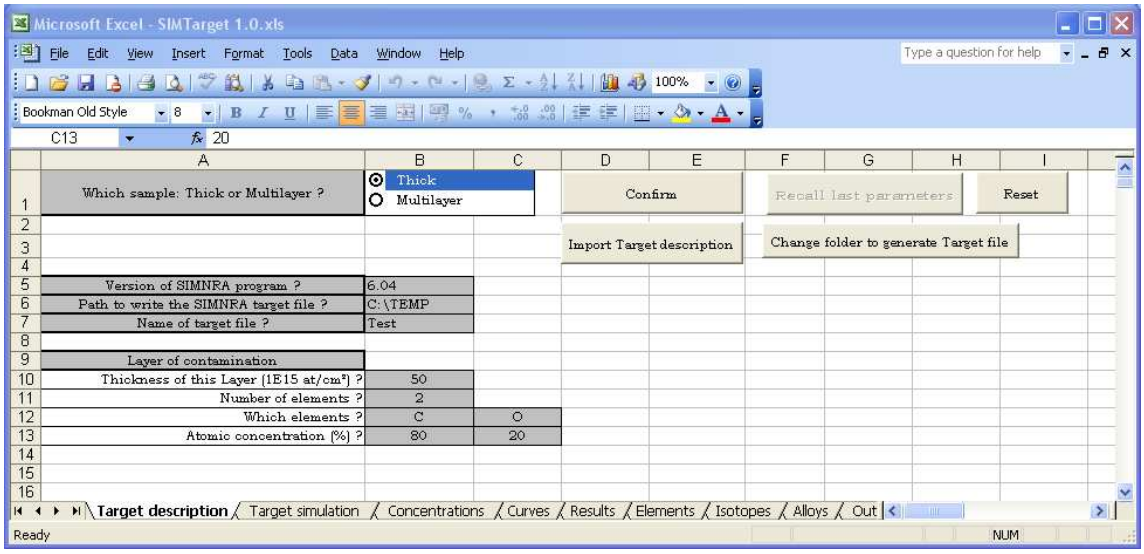


Figure 3: Specification of surface contamination layer.

The SIMTarget code is able to model the diffusion process using a Boltzmann distribution to simulate the transition between two layers (see section 4.1). Select "Boltzmann" in the item list if you wish to model a diffusion process between the surface contamination and the substrate (Figure 4). Otherwise, choose "None". This option will not appear if no layer of contamination has been defined in the previous step. Parameters of the Boltzmann function will be set in the "Target simulation" sheet.

Define the substrate composition as depicted above for the surface contamination.

Gaussian and Lorentzian functions are available to simulate the presence of dopant inside the target (see sections 4.2 and 4.3). Specify the number of dopants desired. For each, set the chemical symbol, the type of curve and the number of curves required. Parameters of these curves will be defined in the "Target simulation" sheet. If no dopant is required, set the number of dopants to 0.

The last step consists of determining the way of slicing the sample in order to generate the SIMNRA target file. It is possible to define different sections which can be sliced into different thicknesses. Therefore, very thin slices can be chosen where the sample composition changes significantly (i.e. around the interface between two layers) and thicker slices can be used everywhere else (Figure 4). Note that, if the thickness of the contamination layer is not divisible by the thickness chosen to slice the sample, SIMTarget adapts the thickness of the last slice automatically, in order to preserve the specified thickness of the contamination layer. For example, if a layer of contamination of 160×10^{15} at.cm^{-2} has to be sliced in slices of 30×10^{15} at.cm^{-2}, the layer will be sliced into four slices of 30×10^{15} at.cm^{-2} and one of

40×10^{15} at.cm^{-2}. Note also that the SIMNRA program does not accept a target file containing more than 102 layers: A dialog box will warn you if this number is exceeded. In this case, the target file is not generated and the requested method of slicing the sample has to be adapted in order to reduce the number of slices.

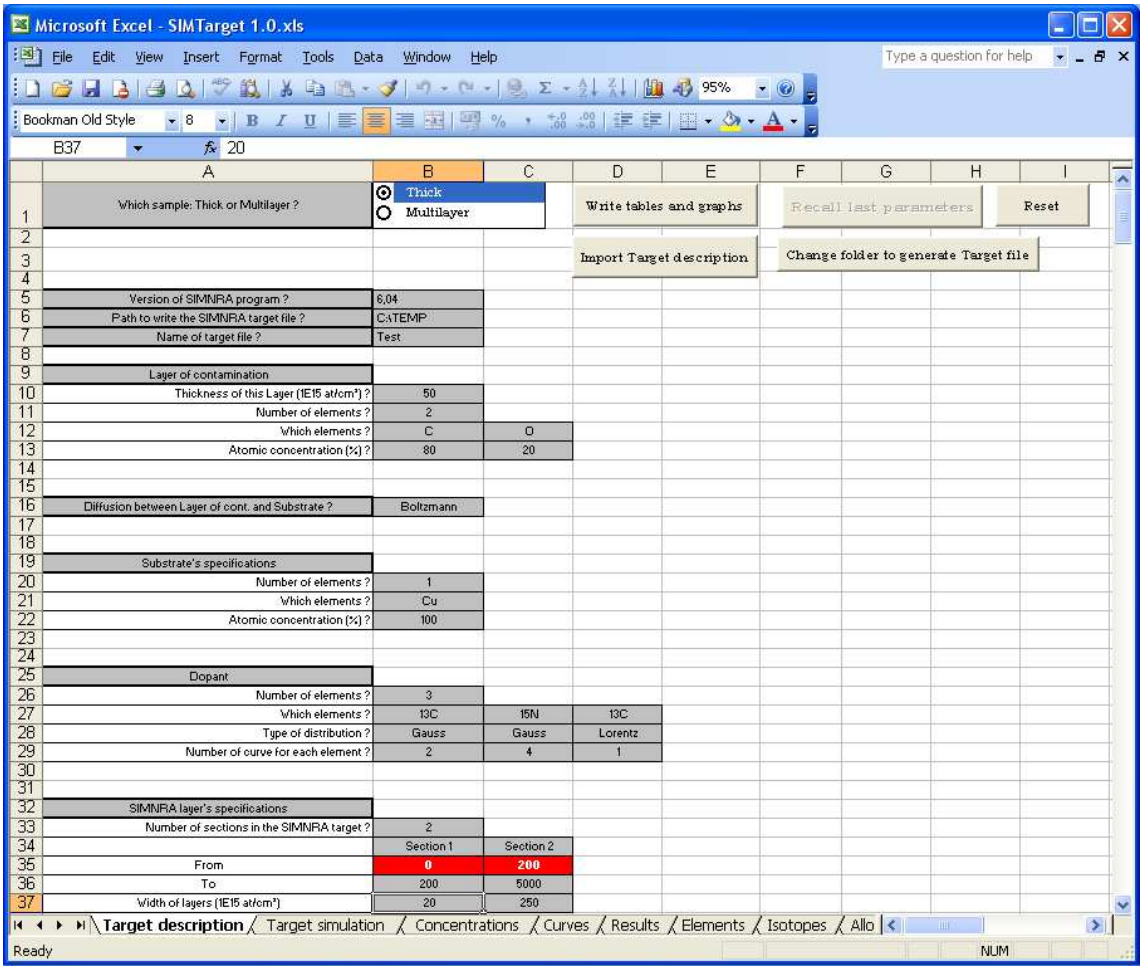


Figure 4: Specifying the diffusion process, substrate composition, dopant and method of slicing the sample.

When the target description is completed, press the "Write tables and graphs" button. This saves the target description in the "Output parameters" sheet and the page layout of all sheets is updated. A new sheet is also created for each dopant in order to show the depth distribution of each Gaussian and Lorentzian curve, which is very convenient for adjusting the parameters of these curves during the target simulation. Finally, the "Simulation target" sheet is activated, and ready to generate the SIMNRA target file.

3.2.2 Multilayer samples

Insert the thickness and the number of element of the layer of contamination (Figure 5). Specify the nature of each element by writing its chemical symbol with the keyboard. A dialog box will warn you if the element or the isotope chosen is not available in the SIMNRA code. Alloys can also be used if they have previously been defined in the "Alloys" sheet (see section 3.5.2). If the surface contamination contains several elements, the concentration of the last constituent will be automatically determined by the program. If no layer of contamination is required, set the thickness and the number of elements to 0.

Set the number of deposited layers and the number of stacked multilayers. The number of stack allows to repeat several times the deposited layers in order to model the stacking of multilayers on a substrate (see example in section 5.3). A single coating is then achieved by choosing only one deposited layer in a single stack (see example in section 5.2). When the description of layer of contamination and structure of deposited layers is completed, press the "Confirm" button.

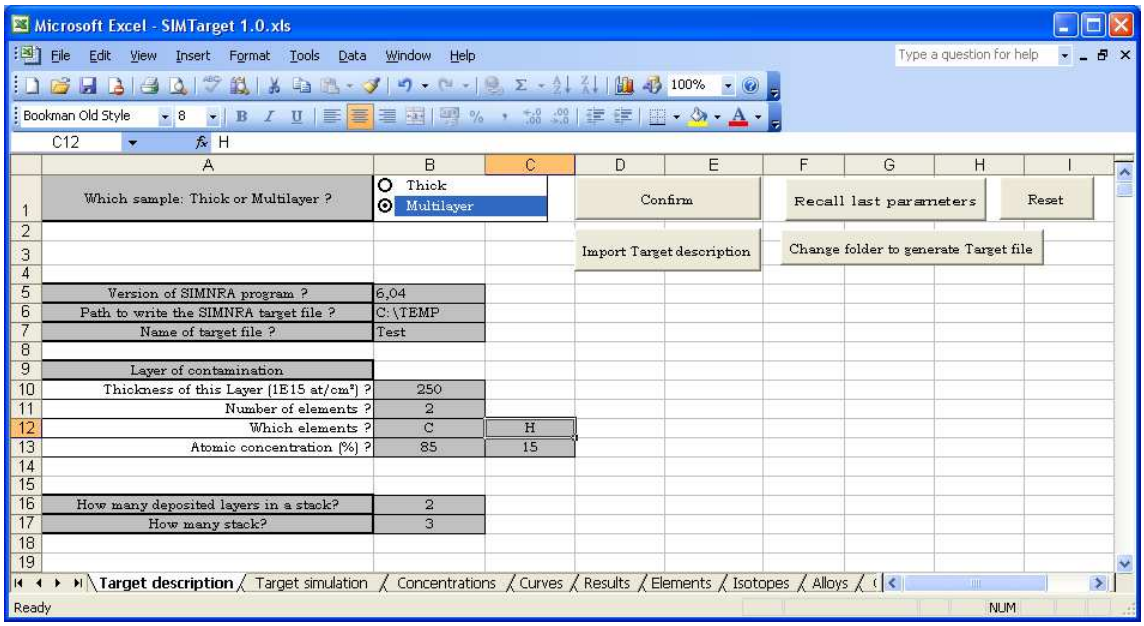

Microsoft Excel - SIMTarget 1.0.xls
File Edit View Insert Format Tools Data Window Help
Type a question for help
Bookman Old Style 8
C12 H
Which sample: Thick or Multilayer ?
Thick
Multilayer
Confirm
Recall last parameters
Reset
Import Target description
Change folder to generate Target file
Version of SIMNRA program ? 6,04
Path to write the SIMNRA target file ? C:\TEMP
Name of target file ? Test
Layer of contamination
Thickness of this Layer (1E15 at/cm²) ? 250
Number of elements ? 2
Which elements ? C H
Atomic concentration (%) ? 85 15
How many deposited layers in a stack? 2
How many stack? 3
Target description Target simulation Concentrations Curves Results Elements Isotopes Alloys
Ready
NUM

Figure 5: Description of the contamination layer and specification of the multilayer structure.

Define the composition of deposited layers, as described above for the layer of contamination, for as many layers as necessary (Figure 6).

SIMTarget code is able to model the diffusion process using a Boltzmann distribution to carry out the transition between two layers (see section 4.1). For each interface, select "Boltzmann" in the item list if you wish to model a diffusion process. Otherwise, select "None". Parameters of the Boltzmann function will be set in the "Target simulation" sheet.

Define the substrate composition as described above for the layer of contamination.

Gaussian and Lorentzian functions are available to simulate the presence of dopants inside the target (see sections 4.2 and 4.3). Specify the number of dopants desired. For each one, specify the chemical symbol, the type of curve and the number of curves required. Parameters of these curves will be defined in the "Target simulation" sheet. If no dopant is required, set the number of dopants to 0.

The last step consists of determining the way of slicing the sample in order to generate the SIMNRA target file. It is possible to define different sections which can be sliced into different thicknesses. Therefore, very thin slices can be chosen where the sample composition changes significantly (i.e. around the interface between two layers) and thicker slices can be used everywhere else. Note that, if the thickness of the contamination layer is not divisible by the thickness chosen to slice the sample, SIMTarget adapts the thickness of the last slice automatically, in order to preserve the specified thickness of the contamination layer. For example, if a layer of contamination of 160×10^{15} at.cm^{-2} has to be sliced in slices of 30×10^{15} at.cm^{-2}, the layer will be sliced into four slices of 30×10^{15} at.cm^{-2} and one of 40×10^{15} at.cm^{-2}. Note also that the SIMNRA program does not accept a target file containing more than 102 layers: A dialog box will warn you if this number is exceeded. In this case, the target file is not generated and the requested method of slicing the sample has to be adapted in order to reduce the number of slices.

When the target description is completed, press the "Write tables and graphs" button. This saves the target description in the "Output parameters" sheet and the page layout of all sheets is updated. A new sheet is also created for each dopant in order to show the depth distribution of each Gaussian and Lorentzian curve, which is very convenient for adjusting the parameters of these curves during the target simulation. Finally, the "Simulation target" sheet is activated, and ready to generate the SIMNRA target file.

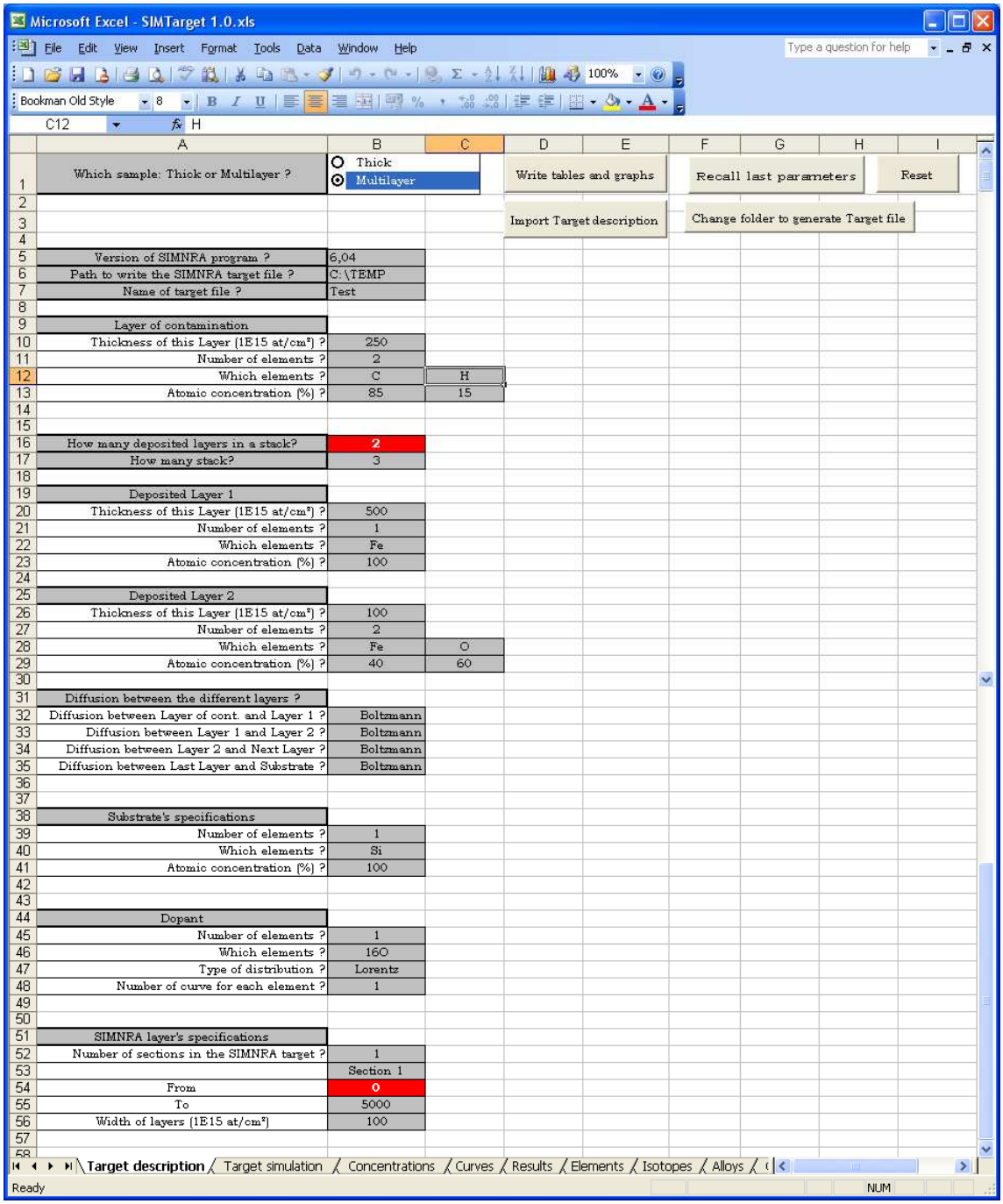

Microsoft Excel - SIMTarget 1.0.xls
File Edit View Insert Format Tools Data Window Help
Type a question for help
Bookman Old Style 8
C12 H
Which sample: Thick or Multilayer ?
Thick
Multilayer
Write tables and graphs
Recall last parameters
Reset
Import Target description
Change folder to generate Target file
Version of SIMNRA program ? 6,04
Path to write the SIMNRA target file ? C:\TEMP
Name of target file ? Test
Layer of contamination
Thickness of this Layer (1E15 at/cm²) ? 250
Number of elements ? 2
Which elements ? C H
Atomic concentration (%) ? 85 15
How many deposited layers in a stack? 2
How many stack? 3
Deposited Layer 1
Thickness of this Layer (1E15 at/cm²) ? 500
Number of elements ? 1
Which elements ? Fe
Atomic concentration (%) ? 100
Deposited Layer 2
Thickness of this Layer (1E15 at/cm²) ? 100
Number of elements ? 2
Which elements ? Fe O
Atomic concentration (%) ? 40 60
Diffusion between the different layers ?
Diffusion between Layer of cont. and Layer 1 ? Boltzmann
Diffusion between Layer 1 and Layer 2 ? Boltzmann
Diffusion between Layer 2 and Next Layer ? Boltzmann
Diffusion between Last Layer and Substrate ? Boltzmann
Substrate's specifications
Number of elements ? 1
Which elements ? Si
Atomic concentration (%) ? 100
Dopant
Number of elements ? 1
Which elements ? 16O
Type of distribution ? Lorentz
Number of curve for each element ? 1
SIMNRA layer's specifications
Number of sections in the SIMNRA target ? 1
Section 1
From 0
To 5000
Width of layers (1E15 at/cm²) 100
Target description Target simulation Concentrations Curves Results Elements Isotopes Alloys
Ready
NUM

Figure 6: Specification of deposited layers composition, diffusion process, substrate composition, dopant and way of slicing the sample.

3.3 *Generation of the SIMNRA target file*

The sample described in section 3.2.1 is used here, in order to show how the routine generates the target file. At the end of the target description, the layout of all SIMTarget sheets is updated and the "Target simulation" sheet is ready to generate the target file. Tables showing the Gaussian, Lorentzian and Boltzmann parameters (all initialised to 0) are presented in this sheet. Set the desired values for these parameters and press the "Create SIMNRA target" button (Figure 7).

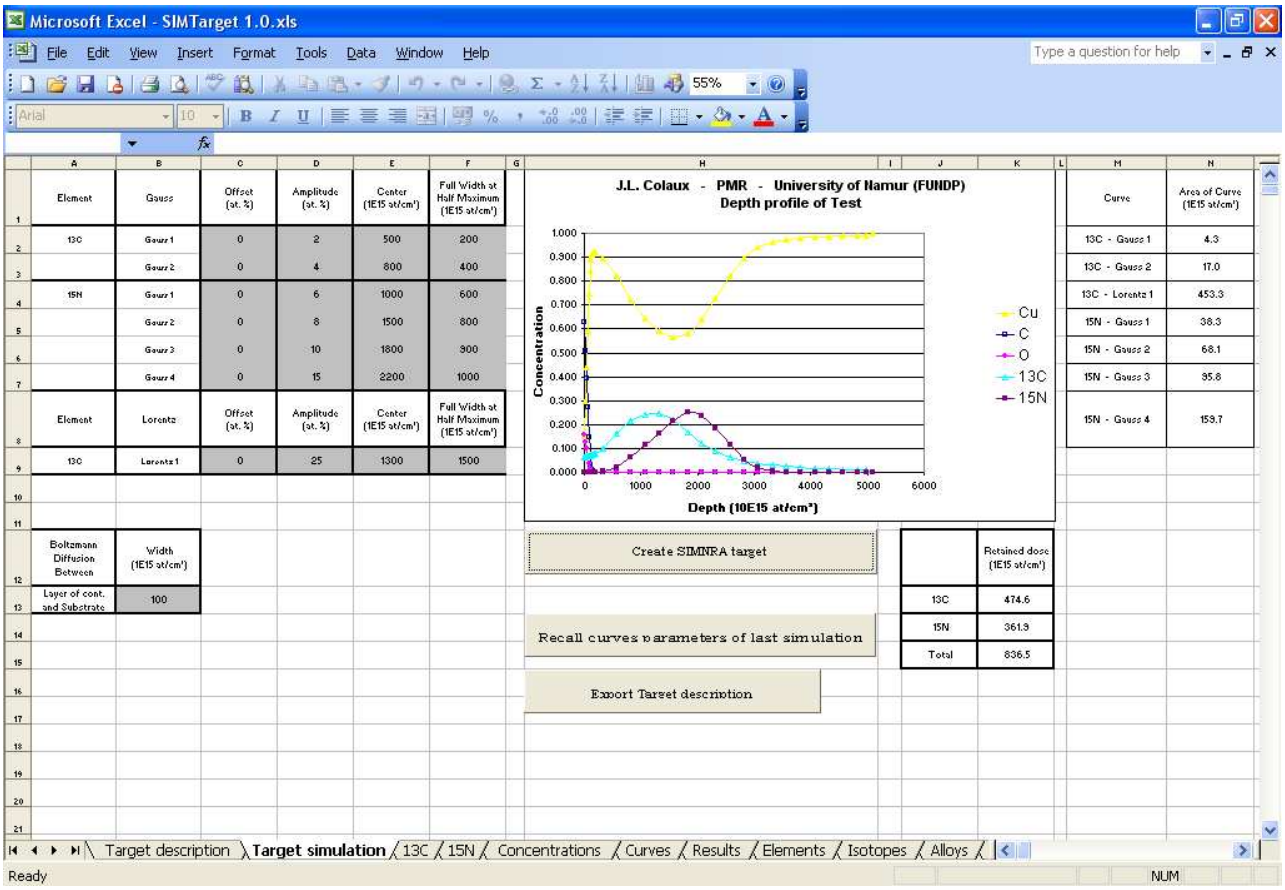


Figure 7: Example of SIMNRA target generation.

When the "Create SIMNRA target" button is pressed, the depth distribution of each target element is calculated and the results are presented in a graph in the "Simulation target" sheet. In this graph, the depth profile of each dopant is obtained to sum the contribution of each Gaussian and Lorentzian curve. These curves are plotted in the sheets named after the different dopants in order to visualise their influence on the target composition (Figure 8).

The retained dose (expressed in 10^{15} at.cm^{-2}) is calculated for each dopant and presented in a table below the graph (Figure 7). The integral of each Gaussian and Lorentzian curve can also be found in a table shown at the right of this general graph. Finally, the SIMNRA target file is generated in the path filename specified in "Target description" sheet.

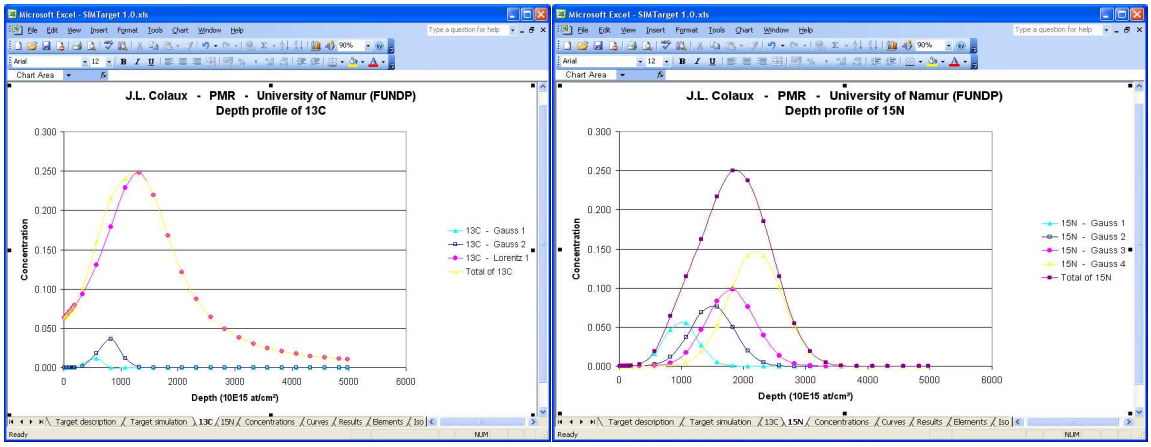

J.L. Colaux - PMR - University of Namur (FUNDP)
Depth profile of 13C
Concentration
Depth (10E15 at/cm²)
13C - Gauss 1
13C - Gauss 2
13C - Lorentz 1
Total of 13C
J.L. Colaux - PMR - University of Namur (FUNDP)
Depth profile of 15N
Concentration
Depth (10E15 at/cm²)
15N - Gauss 1
15N - Gauss 2
15N - Gauss 3
15N - Gauss 4
Total of 15N

Figure 8: Depth profiles of ^{13}C and ^{15}N showing the contribution of each Gaussian and Lorentzian curves.

The target file is directly readable in SIMNRA code in order to simulate the experimental spectrum under analysis. According to the quality of this simulation, users can adapt the target parameters in SIMTarget code, pressing the "Create SIMNRA target" button each time to re-write the code. The depth profile of each element is computed again and the SIMNRA target file is overwritten with the new target composition. Load this file in the SIMNRA program and run it again. Several iterations between SIMTarget and SIMNRA codes may be necessary to obtain good agreement between the experimental and simulated spectra.

Note that, in addition to the parameters shown in the "Target simulation" sheet, some parameters remain adjustable in the "Target description" sheet (i.e. Thickness of different layers; Atomic concentration of elements; methods to slice the sample…). These parameters appear in grey cells in the "Target description" sheet. The unavailable parameters (i.e. Nature of elements; Number of dopants…) appear in red cells. If a modification of these unavailable parameters is required, the program has to be reset by clicking the "Reset" button on the "Target description" sheet. In this case, the "Recall last parameters" button can be very useful to avoid having to re-enter all the target description data manually. The parameters of

Boltzmann, Gaussian and Lorentzian curves can also be recalled using the “Recall curves parameters of last simulation” button in the “Target simulation” sheet.

3.4 *Export / Import of the target description*

As mentioned in the previous section, the “Recall last parameters” and “Recall curves parameters of last simulation” buttons are very useful to avoid having to re-enter all the target description data manually when the target description has to be reset. However, these buttons can only recall the parameters of the last target generated by the SIMTarget code. Due to this limitation, a function to export the complete target description, in order to recall it later, has been provided.

When the agreement between the experimental spectrum and the curve simulated by SIMNRA is considered to be sufficient, hit the “Export Target description” button in the “Target simulation” sheet. The complete description of the target is then written in a text file (typical size ~20kb). The name and the directory of this file are identical to that chosen for the SIMNRA target file.

In order to import a target description, reset the SIMTarget program by hitting the “Reset” button in the “Target description” sheet. Then, click the “Import Target description” button. A dialog box simulating Windows Explorer is opened, in order to select the file to import (Figure 9). Select the required text file and click “open”. The target description is then automatically loaded into the program. All curves and diffusion parameters are automatically recalled and the “Target simulation” sheet is activated and ready to generate a target file. A dialog box will also prompt you to change the name or the directory of the target file in order to avoid overwriting the existing files.

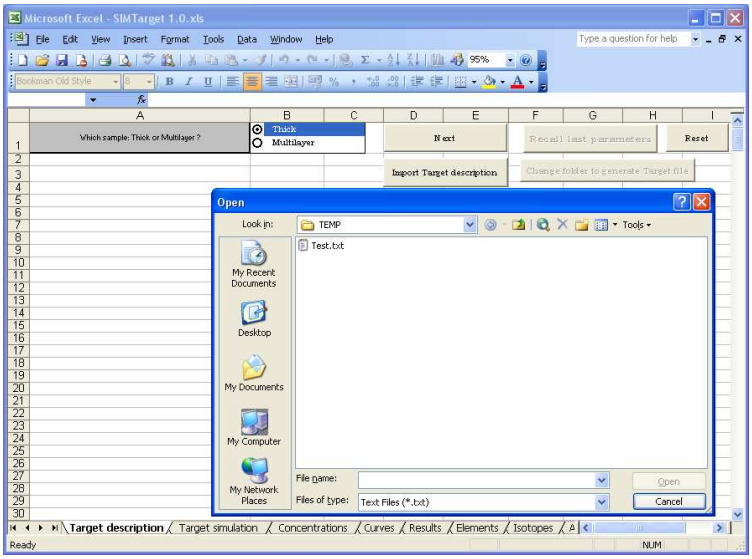


Figure 9: Import a target description file.

3.5 ***Extra tools***

3.5.1 Concentrations sheet

When the sample contains dopants, it may be interesting to determine their average concentration in a specific range. The "Concentration" sheet allows users to calculate this average concentration between depths x_1 and x_2, as set by the user in a text box (Figure 10). The retained dose of each dopant is also determined by the program in the same range. Figure 10 presents the results obtained for the sample described in the section 3.2.1 for a range covering all the sample (left) or centred around the maxima of ^{13}C and ^{15}N depth distributions (right). Note that the retained doses calculated in the first case (left part of Figure 10) are equal to the retained doses displayed on the "Target simulation" sheet (Figure 7).

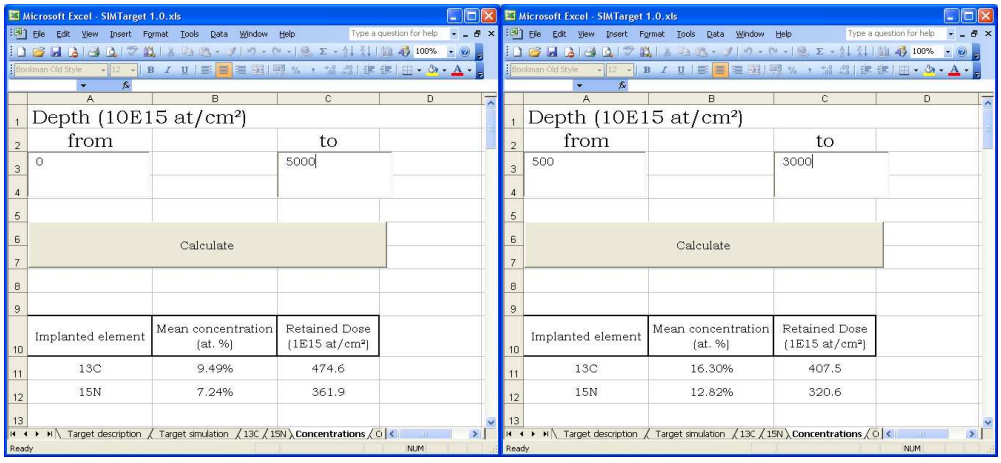


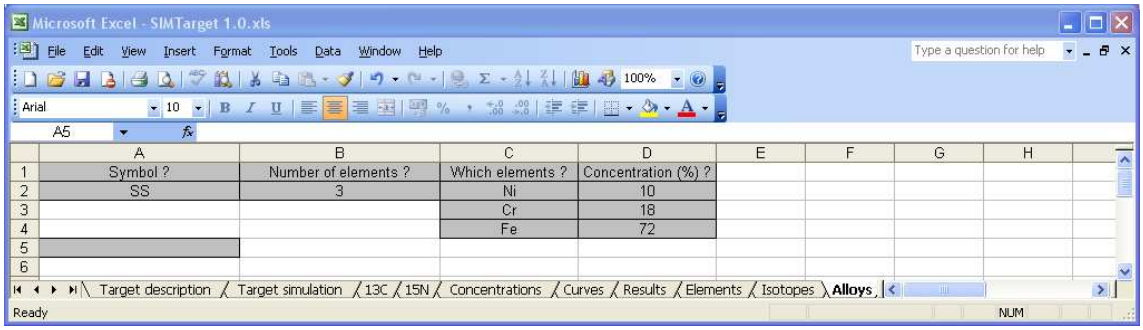
Figure 10: Mean concentration and retained dose calculated for sample described in the section 3.2.1 and for two different ranges.

3.5.2 Alloys sheet

This interactive sheet allows users to define different alloys which will be assumed by the SIMTarget code to be treated as a single element. This alloy will be replaced in the SIMNRA target file by its constituent elements, taking into account the concentration specified in the "Alloys" sheet, during the SIMNRA target file generation. This option is

particularly interesting when the user wishes to adjust the concentration of an alloy in a deposited layer (see example in section 5.2).

Choose a symbol in order to define a new alloy. A dialog box will warn you if the symbol chosen is already used in the “Elements”, “Isotopes” or “Alloys” sheets. In this case, you have to change the symbol. Give the number of elements contained in the alloy. According to this number, new grey cells will appear allowing you to define the nature and the concentration of each element. All elements and isotopes available in the SIMNRA code can be used. The concentration of the last constituent element is automatically determined by the program.


Microsoft Excel - SIMTarget 1.0.xls
File Edit View Insert Format Tools Data Window Help
Type a question for help
100%
Arial 10
A5
Target description Target simulation 13C 15N Concentrations Curves Results Elements Isotopes Alloys
Ready
NUM

	A	B	C	D	E	F	G	H
1	Symbol ?	Number of elements ?	Which elements ?	Concentration (%) ?				
2	SS	3	Ni	10				
3			Cr	18				
4			Fe	72				
5								
6								

Figure 11: Definition of the stainless steel composition.

4 Computational approach

The SIMRA target file is generated when the sample structure has been comprehensively defined. For this purpose, the code determines the analytical depth profile of each element of the sample. The sample is then sliced as describe in the “Target description” sheet (see section 3.2) and a very simple algorithm determines the mean composition of each sample slice. The results are then plotted in SIMTarget and written in the SIMNRA target file. More details about the algorithm used by SIMTarget can be found in reference [3].

In order to understand the meanings of the different curve parameters used in SIMTarget code, a very short description of the Boltzmann, Gaussian and Lorentzian functions is presented below.

4.1 Boltzmann function

The Boltzmann distribution is used to carry out the transition between two layers in order to model the diffusion process. Let us consider an element of which the concentration is A_1 in the *Layer 1* and A_2 in the *Layer 2*. If X_0 is the depth position of the interface between these two layers, the concentration of the element at the depth X is given by,

$$y = \frac{A_1 - A_2}{1 + e^{(X - X_0)/dx}} + A_2$$

where dx is related to the width W of the Boltzmann distribution (Figure 12) by,

$$dx = \frac{W}{2 \times \ln\left[0.9 / (1 - 0.9)\right]}$$

The width of the Boltzmann distribution W is the parameter determined by the user in the SIMTarget code.

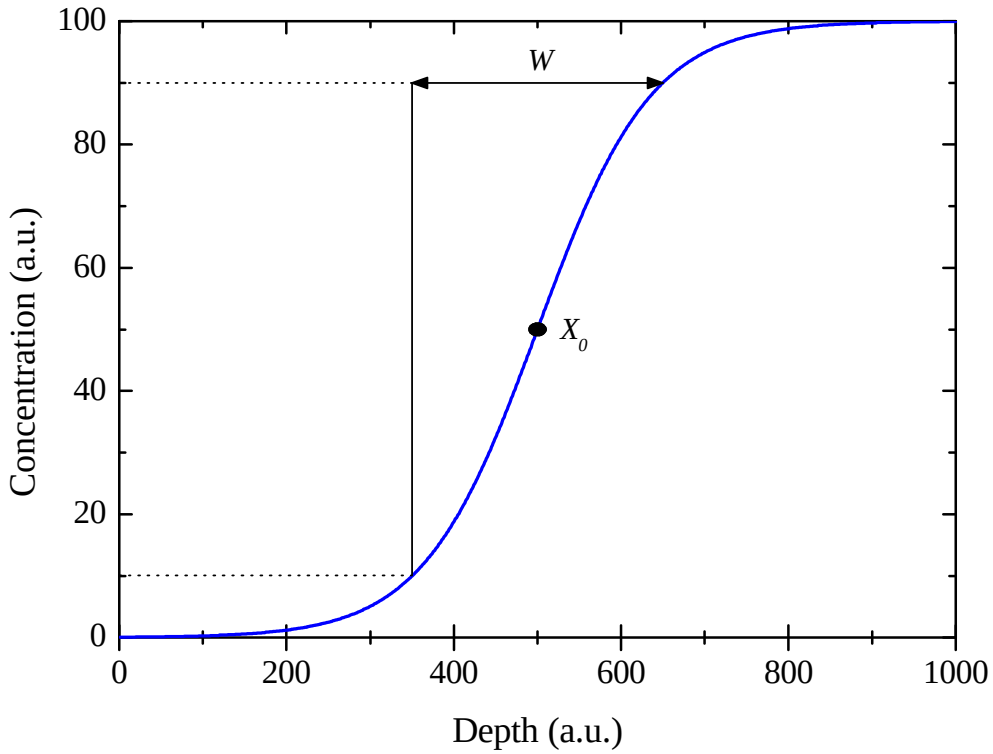


Figure 12: Representation of the Boltzmann function used by SIMTarget to model the diffusion process for $A_1 = 0$, $A_2 = 100$ and $W = 300$.

Note that the use of Boltzmann distribution can lead to a target composition having no physical interpretation. This is the case when the half width of Boltzmann distribution is larger than the thickness of one of the two layers implicated in the diffusion process. In order to understand this phenomenon let us consider a layer of 200×10^{15} at.cm^{-2} of pure carbon deposited on a copper substrate. If a Boltzmann distribution with a width of 500×10^{15} at.cm^{-2} is applied to the interface, we obtain the depth profile of carbon presented in blue in the Figure 13. On this figure, we can clearly observe that the number of carbon atoms having diffused into copper (red surface labelled A_2) is more important than the number of carbon atoms having left the deposited layer (green surface labelled A_1). That means that the integral of the carbon depth profile, equal to 216×10^{15} at.cm^{-2}, is greater than the total amount of carbon initially specified (200×10^{15} at.cm^{-2}).

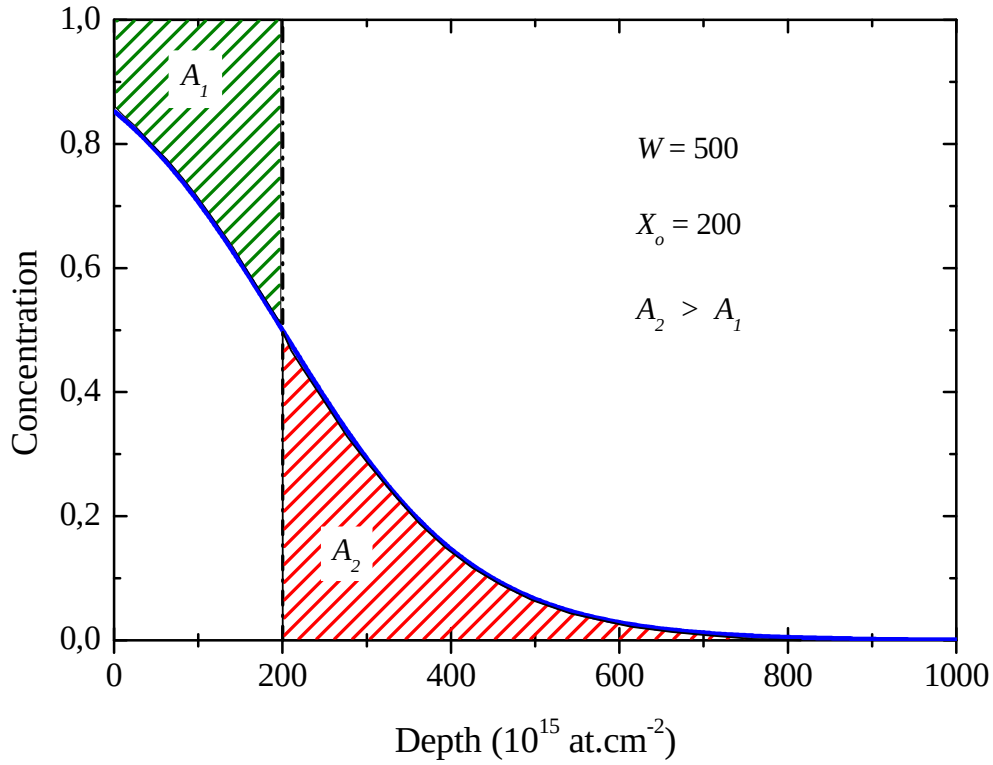


Figure 13: Artefact of the use of Boltzmann distribution.

4.2 Gaussian function

The Gaussian function can be used to model the presence of dopant inside the sample. The concentration of the dopant, *y*, calculated at the depth *X*, is given by:

$$y = y_0 + A\, e^{-\frac{(X - X_o)^2}{2W^2}}$$

where y_0, A and X_0 are the offset, the amplitude and the centre of the Gaussian curve, respectively (Figure 14). W is related to the Full Width at Half Maximum, W_1, of the Gaussian distribution by,

$$W = \frac{W_1}{2 \times \sqrt{\ln(4)}}$$

The offset (y_0), amplitude (A), centre (X_0) and Full Width at Half Maximum (W_1) are the Gaussian parameters determined by the user in the SIMTarget code.

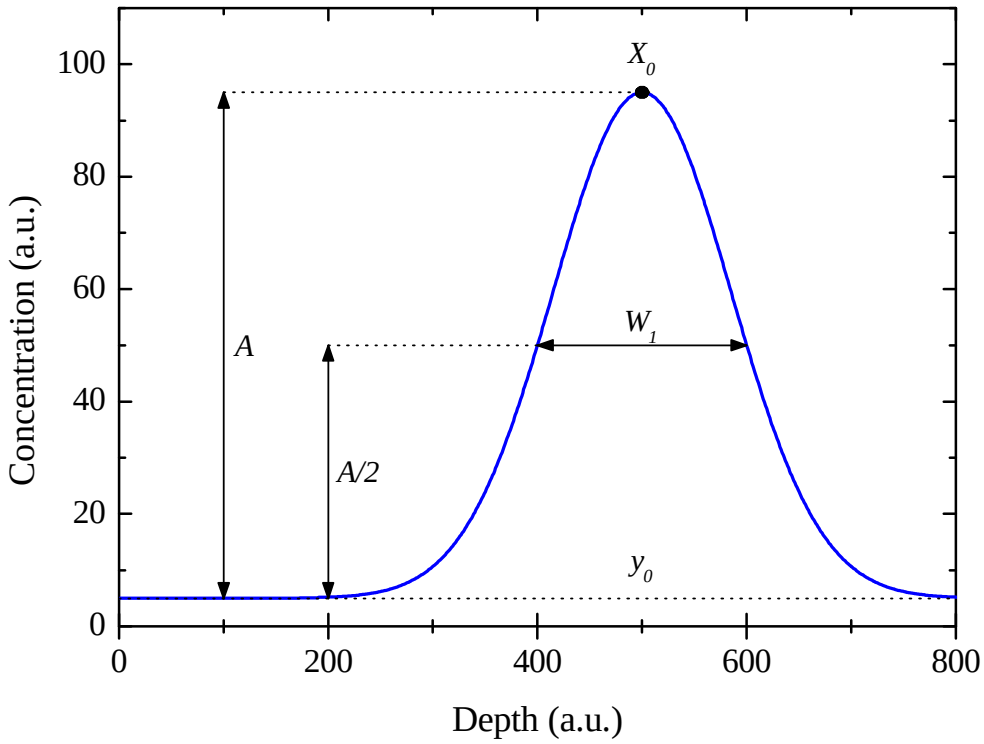


Figure 14: Representation of the Gaussian function used by SIMTarget for y_0 = 5, A = 90 and W_1 = 200.

4.3 Lorentzian function

The Lorentzian function can be used to model the presence of dopant inside the sample. The concentration of the dopant, y, calculated at the depth X, is given in by:

$$y = y_0 + \frac{A W^2}{4(X - X_0)^2 + W^2}$$

where y_0, W, A and X_0 are the offset, the Full Width at Half Maximum, the amplitude and the centre of the Lorentzian curve, respectively (Figure 15).

The offset (y_0), amplitude (A), centre (X_0) and Full Width at Half Maximum (W) are the Lorentzian parameters determined by the user in the SIMTarget code.

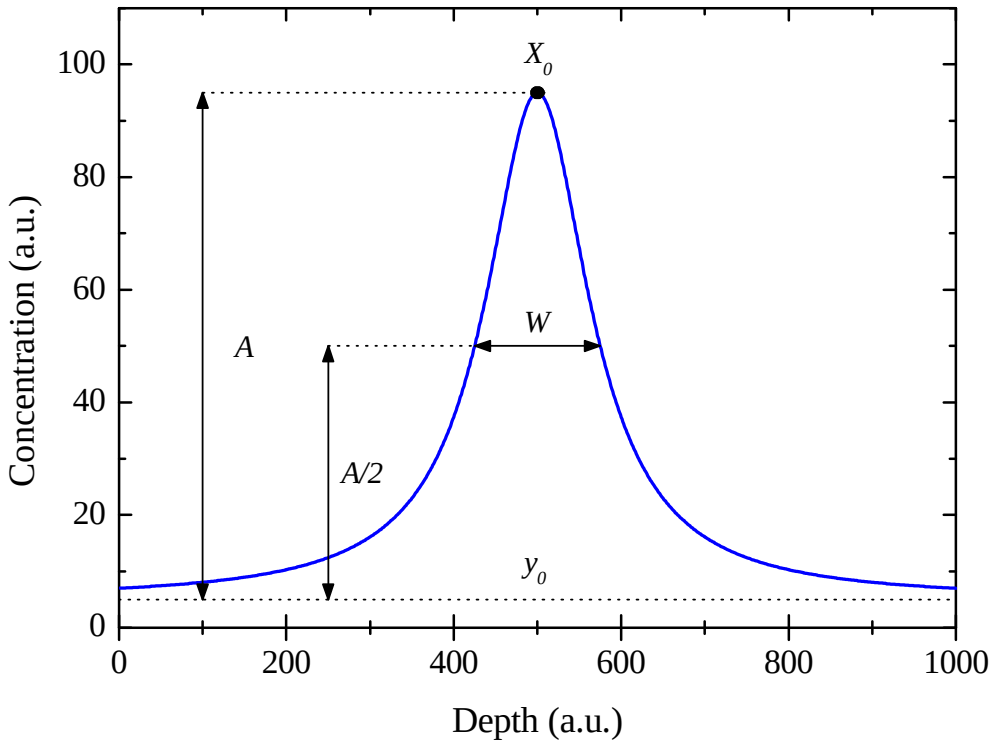


Figure 15: Representation of the Lorentzian function used by for $y_0 = 5$, $A = 90$ and $W_1 = 150$.

5 Examples

Three different applications are presented in order to illustrate the power of the combination of SIMTarget and SIMNRA programs to characterise complex samples by ion beam analysis: Nuclear Reaction Analysis (NRA) of co-implantation of carbon and nitrogen into copper; Non-Rutherford Backscattering Spectroscopy (NBS) of a metallic oxide deposited by physical vapour deposition (PVD) at high temperature; and Rutherford Backscattering Spectroscopy of a multilayer coatings deposited by PVD on a silicon substrate.

The aim of this section is to give an overview of the potential of the SIMTarget code. Thus we simply present the way in which SIMTArget was used to obtain these results. More details about the production of samples and the techniques of analysis can nevertheless be found in a previous work [3].

5.1 NRA of co-implantation of carbon and nitrogen into copper

These samples are polished polycrystalline copper substrates, simultaneously implanted with ^{13}C and ^{14}N using a non-deflected beam line of a 2MV ALTAÏS[1] Tandetron accelerator. Figure 16 shows a typical experimental spectrum recorded at 150° by NRA with a 1.05 MeV incident deuteron beam. The nuclear reactions responsible of the different peaks are indicated on the figure. The simulation was performed with the SIMNRA 6.04 program using nuclear reaction cross sections measured by M. Kokkoris et al. [4], S. Pellegrino et al. [5] and J.L. Colaux et al. [6].

[1] **A**ccélérateur **L**inéaire **T**andetron pour l'**A**nalyse et l'**I**mplantation des **S**olides

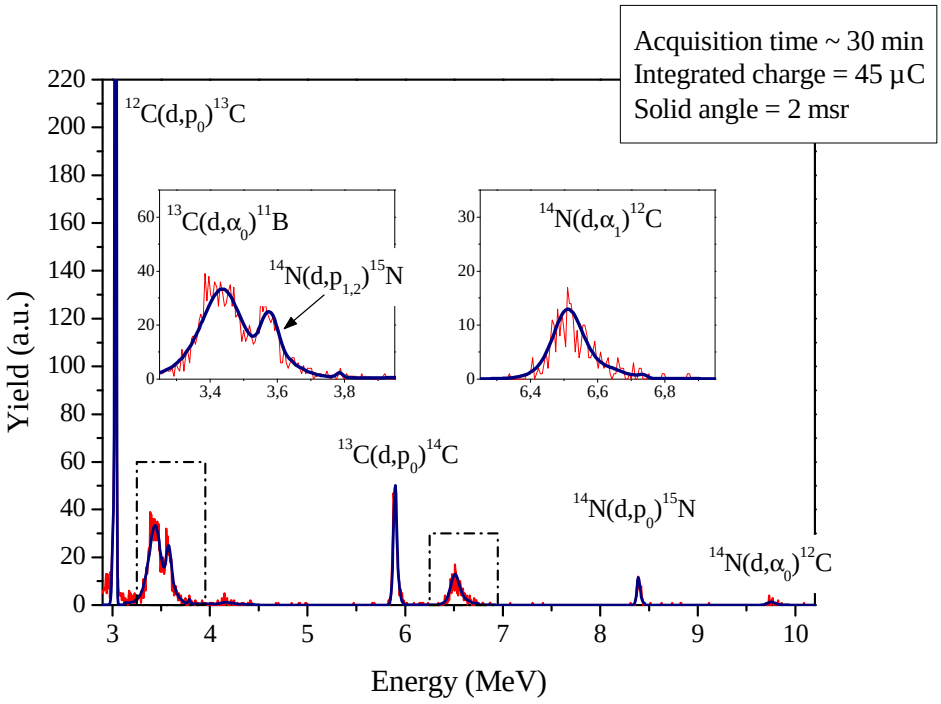


Figure 16: Experimental (red line) and simulated (blue line) NRA spectra recorded at 150° for copper simultaneously implanted with 13C and 14N at room temperature.

The SIMNRA target composition was adjusted using the SIMTarget code in order to obtain the best agreement between the experimental and the simulated spectra (Figure 16). This result was achieved using a thick sample of pure copper. A layer of contamination of 265×10^{15} at.cm^{-2} thick was added to take into account the carbon build-up occurring during the implantation process. A Boltzmann distribution was applied at the interface between carbon contamination and copper in order to model the ion beam mixing with the implantation beam. Eight Gaussian curves were used to model the different carbon and nitrogen ion species (differing charge states) co-implanted into the copper. As the target composition varies very quickly at the interface, the first 1000×10^{15} at.cm^{-2} of the sample were sliced into thin 50×10^{15} at.cm^{-2} layers. The rest of the sample was sliced into layers of 125×10^{15} at.cm^{-2}. The depth profile generated (in less than 10 seconds!) by the SIMTarget code, running on a Pentium (1.60 GHz, 512 Mb of RAM), is presented in Figure 17. Thanks to the very good depth resolution of the (d,α) nuclear reactions, the shape of these depth distributions can directly be observed in the peaks showed in the insets of Figure 16. The carbon and nitrogen depth distributions are shown in more details in Figure 18. As labelled on the figure, each Gaussian curve can be associated with an implanted ion species.

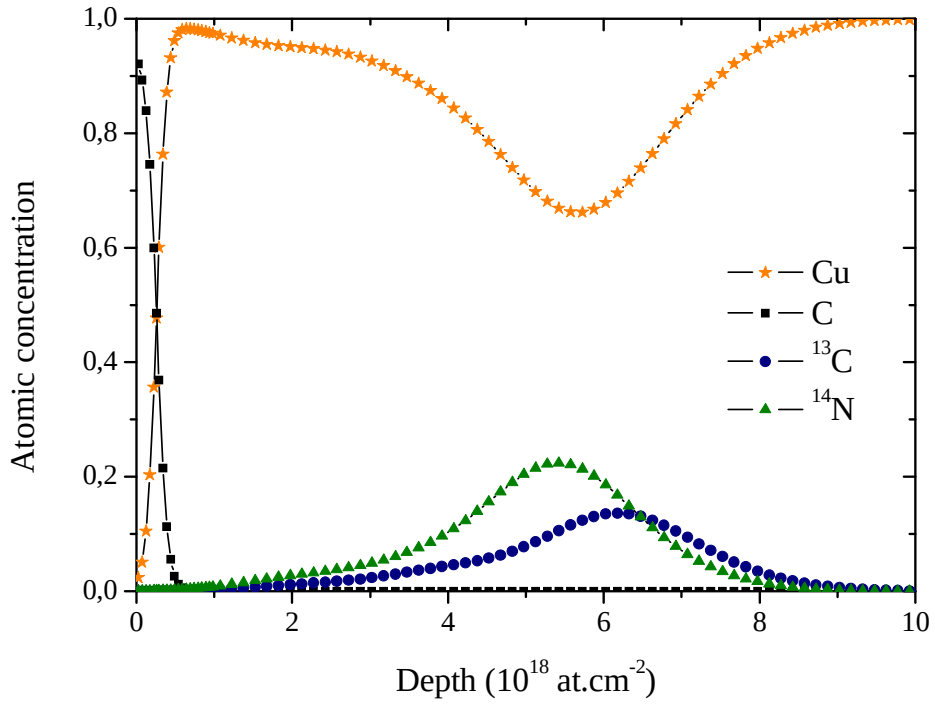


Figure 17: Depth distributions of Cu, C (surface contamination), ^{13}C and ^{14}N generated by SIMTarget code in order to perform the SIMNRA simulation presented in Figure 16.

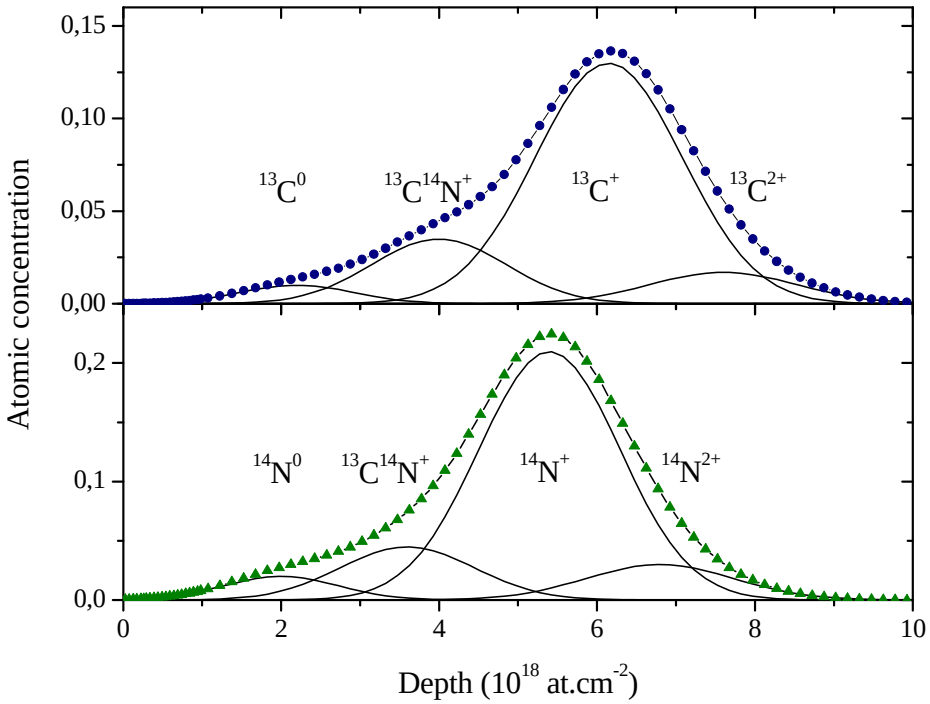


Figure 18: Depth profiles of ^{13}C and ^{14}N generated by the SIMTarget code for the copper sample simultaneously implanted with ^{13}C and ^{14}N at room temperature.

5.2 *NBS of metallic oxides deposited on stainless steel*

Metallic oxide thin film was deposited using reactive DC magnetron sputtering onto polished stainless steel substrate at high temperature (about 400° C). The thickness of the deposited layer was estimated at 200 nm. The sample was characterised by Non-Rutherford Backscattering Spectroscopy using a $^{4}He^{+}$ beam of 3.0 MeV. A typical experimental spectrum recorded at 165° is presented in the Figure 19. Signals from oxygen (O), stainless steel (SS) and metallic element (M) are indicated by arrows on the figure. The simulated curve was calculated by SIMNRA 6.04 code.

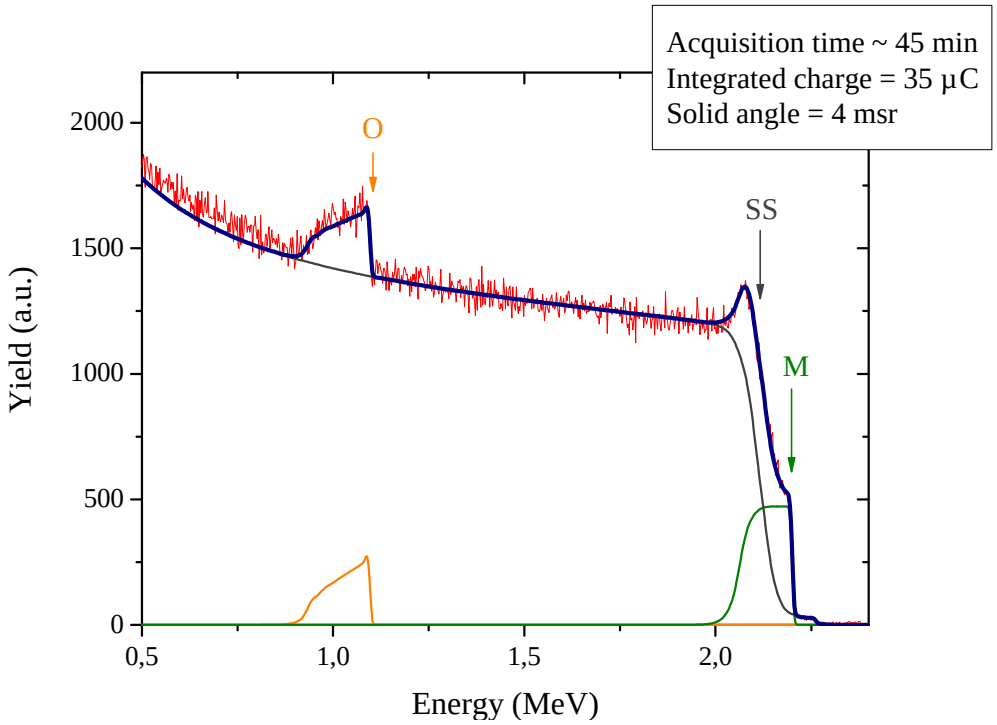


Figure 19: Experimental (red line) and simulated (blue line) NBS spectra recorded at 165° for the metallic oxide deposited onto stainless steel at high temperature.

The sample composition was adjusted using the SIMTarget program. A metallic oxide layer of 1800×10^{15} at.cm^{-2} on a stainless steel substrate was used. The stainless steel diffusion, indicated by the small signal rising up at 2.25 MeV in Figure 19, was modelled by adding 2.6 atomic percent of stainless steel inside the deposited layer and by applying a Boltzmann profile at the interface. The diffusion can clearly be observed on the simulated elemental spectra shown in thin colour lines in Figure 19. A Lorentzian distribution of oxygen

centred on 1900 $\times$ 10^{15} at.cm^{-2} was added in order to model the substrate oxidation occurring prior to the deposition process. The target depth profile sliced into layers of 70 $\times$ 10^{15} at.cm^{-2} is shown in Figure 20. Its generation took less than 5 seconds with the SIMTarget code running on a Pentium (1.60 GHz, 512 Mb of RAM). Note that the transition between deposited layer and substrate does not look like a Boltzmann distribution due to the presence of the Lorentzian distribution [3].

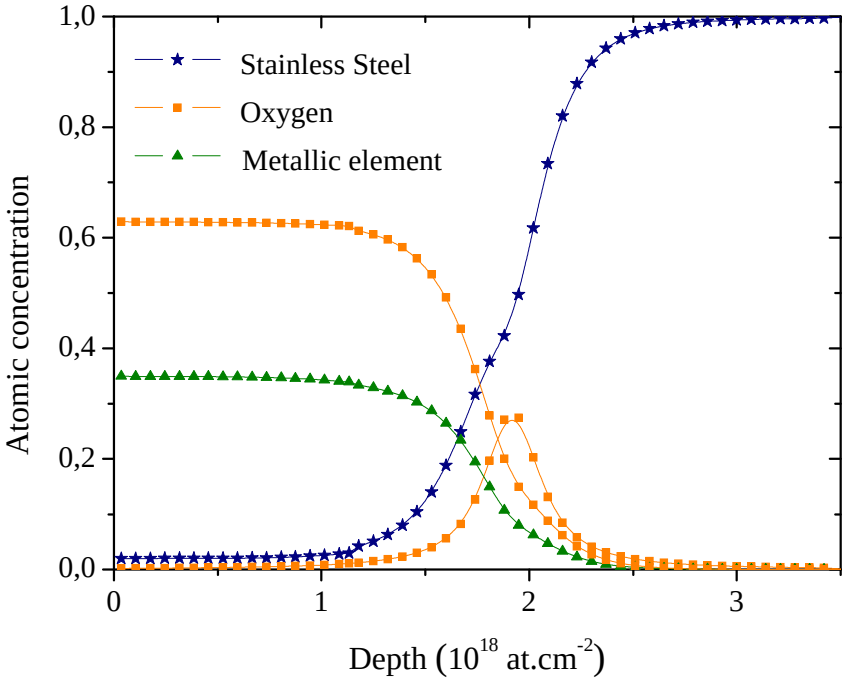


Figure 20: Depth distributions of stainless steel (SS), metallic element (M) and oxygen (O) generated by SIMTarget code in order to perform the SIMNRA simulation presented in Figure 19.

5.3 ***RBS of multilayer coatings deposited on carbon***

SIMTarget and SIMNRA codes can be also used to determine the best experimental setup, allowing characterisation of more complex samples such as a stacked multilayer. We present here the case of five FeN/Fe_2O_3 bi-layers deposited onto carbon.

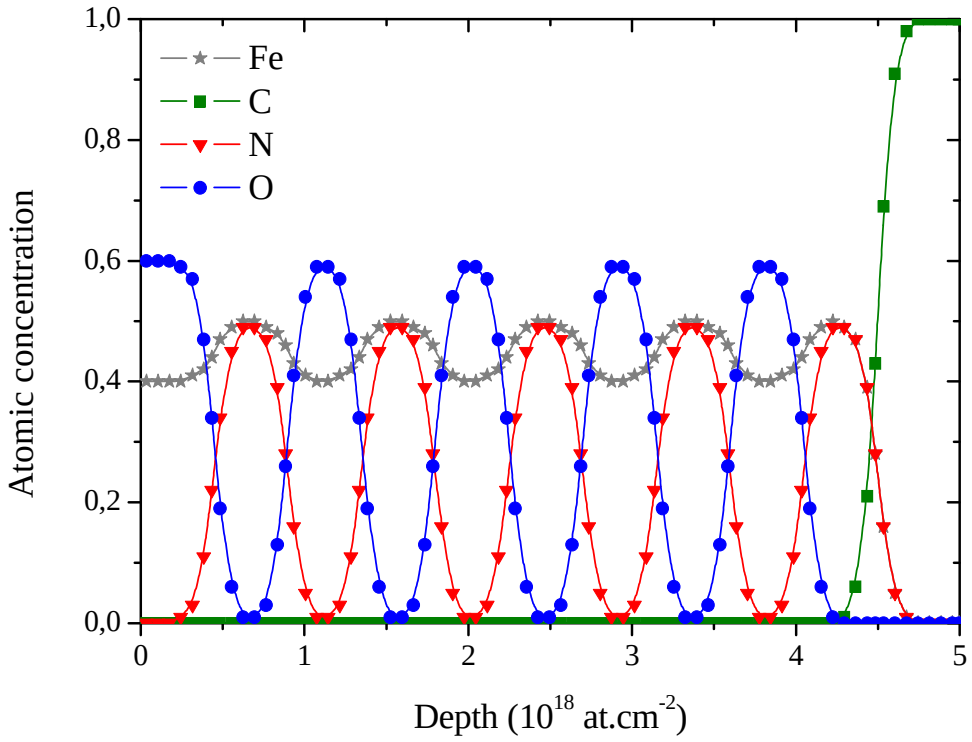


Figure 21: Depth distributions of carbon, iron, nitrogen and oxygen generated by SIMTarget to model the Fe_2O_3/FeN bi-layers deposited by reactive magnetron sputtering onto a carbon substrate.

The thickness of FeN and Fe_2O_3 layers was fixed at 450×10^{15} at.cm^{-2}, and the transition of each interface was carried out using a Boltzmann distribution with a width of 200×10^{15} at.cm^{-2}. The sample was sliced into layers of 70×10^{15} at.cm^{-2}. The target depth profile was generated in less than 5 seconds with a Pentium (1.60 GHz, 512 Mb of RAM), and is presented in the Figure 21.

The simulated curve obtained for a $^4He^+$ beam of 1.50 MeV hitting the sample at an angle of 30° with respect to the normal of the surface, and a detection angle of 165° is presented in Figure 22. We can observe that the signal of iron is well isolated. The particles

backscattered by the oxygen atoms of the two first bi-layers are also well separated from the rest of the spectrum. This experimental setup should then allow us to characterise the two first bi-layers.

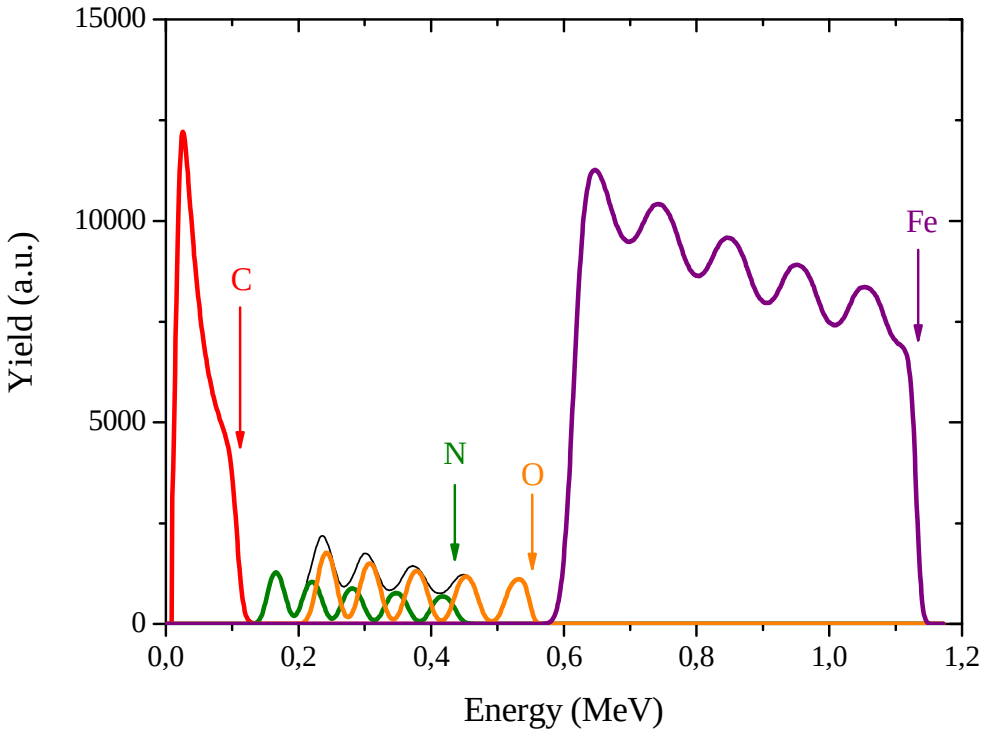


Figure 22: Simulated curves calculated by SIMNRA for the FeN/Fe_2O_3 bi-layers deposited onto a carbon substrate analysed by RBS with an α beam of 1.50 MeV.

6 Acknowledgements

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